Determination of Schottky barriers in 2D heterophase devices.

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The contact-channel resistance is a crucial performance bottleneck in the development of 2D transistor technologies. High Schottky barriers between the contact and channel represent one of the main challenges for reducing the resistance of such devices. In this work, we investigate three different methods for extracting the Schottky barrier; an analysis of the density of states (DOS), the transmission spectrum, and the temperature dependence of the current. Electronic structure calculations commonly apply one of the first two methods, which is based on electrostatic profiles, whereas the latter is often used experimentally. We use Density Functional Theory calculations and the non-equilibrium Green's function method to compare the three methods. We investigate the charge transport in monolayer $MoTe_2$ 1T'-1H junctions and find that the calculated barriers deviate significantly when comparing the three methods. Our results highlight that non-equilibrium calculations are necessary, if barrier heights from simulations are to be compared with experimental results. We find that for a highly n-doped device, the disagreement between the methods is remarkably large. The barrier height extracted from the temperature variation of the current is 48 meV whereas the height is 0.36 eV when extracting it from the DOS. This sheds some light on the long-standing disagreement between the experimentally measured barriers and the calculated barriers for transition metal dichalcogenide heterophase devices. Experimental measurements using the temperature dependence of the current have shown barriers in the order of tens of meV's[1-2] whereas ab-initio calculations using the DOS have shown barriers in the order of hundreds of meV's.[3-4] Our results suggest that tunneling may dominate the temperature dependence of the current for these devices, which leads to a significant reduction of the measured barrier compared to the barrier seen in the DOS.

References

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[3] Z.Q. Fan et. al., ACS Appl. Mater. Interfaces 10 (2018) 19271.
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Figures

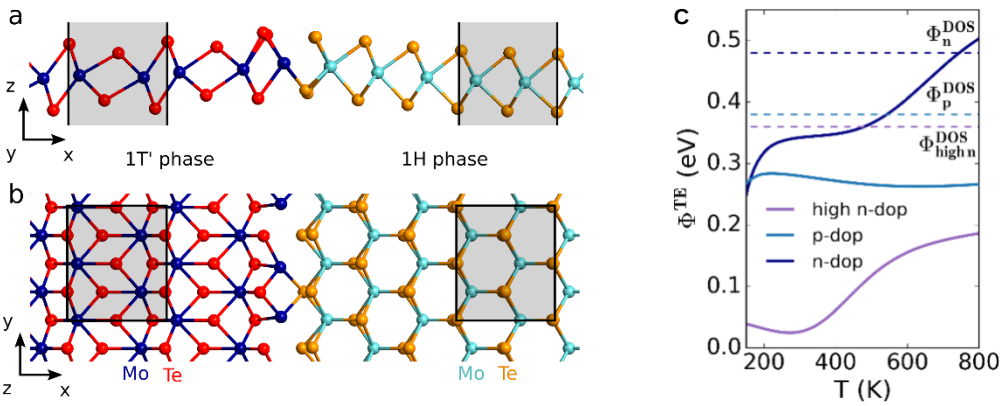

Figure 1: The 1T'-1H interface of ML $MoTe_2$ seen from, **a**, the side and, **b**, the top. **c** shows a comparison between the barrier height determined from the temperature dependence of the current, Φ^{TE}, and the barrier height determined from the DOS, Φ^{DOS}, at different temperatures.